MODELLING AND SIMULATION OF FERMENTATION PRODUCT PURIFICATION USING BATCH

FAEZAH BT BAKAR

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ABSTRACT

Batch distillation has important for industries recent years. This is mainly due to its flexibility and capability to produce high purity product. The simulation of batch distillation columns during steady state operations is a very challenging modelling problem because of the complex dynamic behaviour. In order to verify this issue, simulation of this batch distillation column is to be performed by using computer aided design software and mathematical model so that the results can be validated. This study is required to model and simulate of fermentation product purification using batch distillation. In this study, simple mathematical models are proposed for the simulation of the dynamic behaviour during steady state operations from product of fermentation. Simulation of simple batch distillation was done by using mathematical method and computer simulator, MATLAB ®. The results from these simulations were used as a basis to validate the results obtained from experimentally. As conclusion, distillate and bottoms composition for ethanol drop gradually over time by using graphical method and the trend from simulation showed that the distillate and bottoms composition for ethanol increase and decrease over the time respectively. The declining trend was due to the unsteady state nature of batch distillation, where the lighter component at the bottoms will deplete over time. As using computer software simulation, it able to integrate the model equations for fermentation product purification based on suitable numerical methods and it also gain the understanding due to simulation.

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ABSTRAK

Kebelakangan beberapa tahun ini, penyulingan berkelompok mempunyai kepentingan bagi industri . Hal ini adalah disebabkan oleh fleksibiliti dan keupayaan untuk menghasilkan keaslian produk yang tinggi. Simulasi kolum penyulingan kelompok semasa operasi keadaa mantap adalah masalah pemodelan yang sangat mencabar kerana dalam keadaan dinamik kompleks. Dalam usaha untuk mengesahkan isu ini, simulasi dalam penyulingan kelompok harus dilakukan dengan menggunakan komputer perisian reka bentuk dibantu dan model matematik supaya keputusan boleh disahkan. Kajian ini diperlukan untuk membina model dan simulasi pembersihan produk penapaian menggunakan penyulingan kelompok. Dalam kajian ini, model matematik mudah telah dicadangkan untuk simulasi kelakuan dinamik semasa operasi keadaan mantap daripada hasil penapaian. Simulasi penyulingan kelompok telah dilakukan dengan menggunakan kaedah matematik dan simulator komputer, MATLAB ®. Keputusan daripada simulasi ini telah digunakan sebagai asas untuk mengesahkan keputusan yang diperolehi daripada eksperimen. Kesimpulannya, hasil sulingan etanol dan hasil etanol dalam bekas pemanas adalah turun secara beransur-ansur dari semasa ke semasa dengan menggunakan kaedah graf dan trend daripada simulasi menunjukkan bahawa komposisi sulingan dan etanol dalam pemanas bagi etanol masing-masing adalah meningkat dan berkurangan dari masa ke masa itu. Hal ini oleh sifat keadaan tak mantap kumpulan penyulingan, di mana komponen ringan di dalam pemanas akan berkurang apabila lebih masa.Dengan menggunakan simulasi komputer perisian, ia dapat mengintegrasikan persamaan model untuk pembersihan produk penapaian berdasarkan kaedah berangka dan ia juga mendapat kefahaman kerana simulasi.

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A and n: regression coefficient for chemical compound respectively

H Enthalpy of vaporisation, KJ/mol

H_e enthalpy of vaporisation of ethanol, KJ/mol

H_w enthalpy of vaporisation of water, KJ/mol]

Lo Initial charge, kmol

Lo initial charge, mol

Lt total holdup at bottom at any time, kmol

Lt Total holdup at bottom at any time, kmol

Q heat input, KW

R Reflux ratio

T Temperature, K

Tc Critical temperature, K

V *vapour* boil-up rate, kmol/s

x_e mole fraction of ethanol, mole

x_o Initial bottom composition of lighter component

x_t Bottom composition of lighter component at any time

x_w Distillate mole fraction of water

CHAPTER 1

INTRODUCTION

1.1 Introduction

Batch distillation process is an important separation technique for many centuries that used in many areas of pharmaceutical and especially in chemical industries. It uses for separating or purifying liquid mixtures and waste removal in chemical process industries. Fermentation is one of the chemical processes in this industry. Where, local vinegar is formed from fermentation that can be used for separating via simulation. Therefore, it has common issues for the researchers in order to design alternative and suitable column configurations, to develop of mathematical models in line with the development of numerical methods and to use of artificial software networks in dynamic modelling, optimisation and control

In addition, batch distillation processes can easily handle variations both in the feed composition and in the product specifications. This variation of batch distillation processes provides the ability to manage with a market characterized by short product life times and strict specification requirements. Although the fixed cost required for constructing a batch column is lower than a series of continuous column, but the operating costs of batch distillation is higher due to more energy consumption. Furthermore, the lowest capital cost design does not necessarily make for the most economical solution due to the low performance and high operating costs associated with a high reflux column (Kian & Sorensen, 2012). Since, batch distillation is often attractive for fermentation product purification. The flexibility of batch distillation allow for configuring the column of conventional column (used in this study), inverted column, middle vessel column and multi-vessel column, which are given in Figure 1.1.

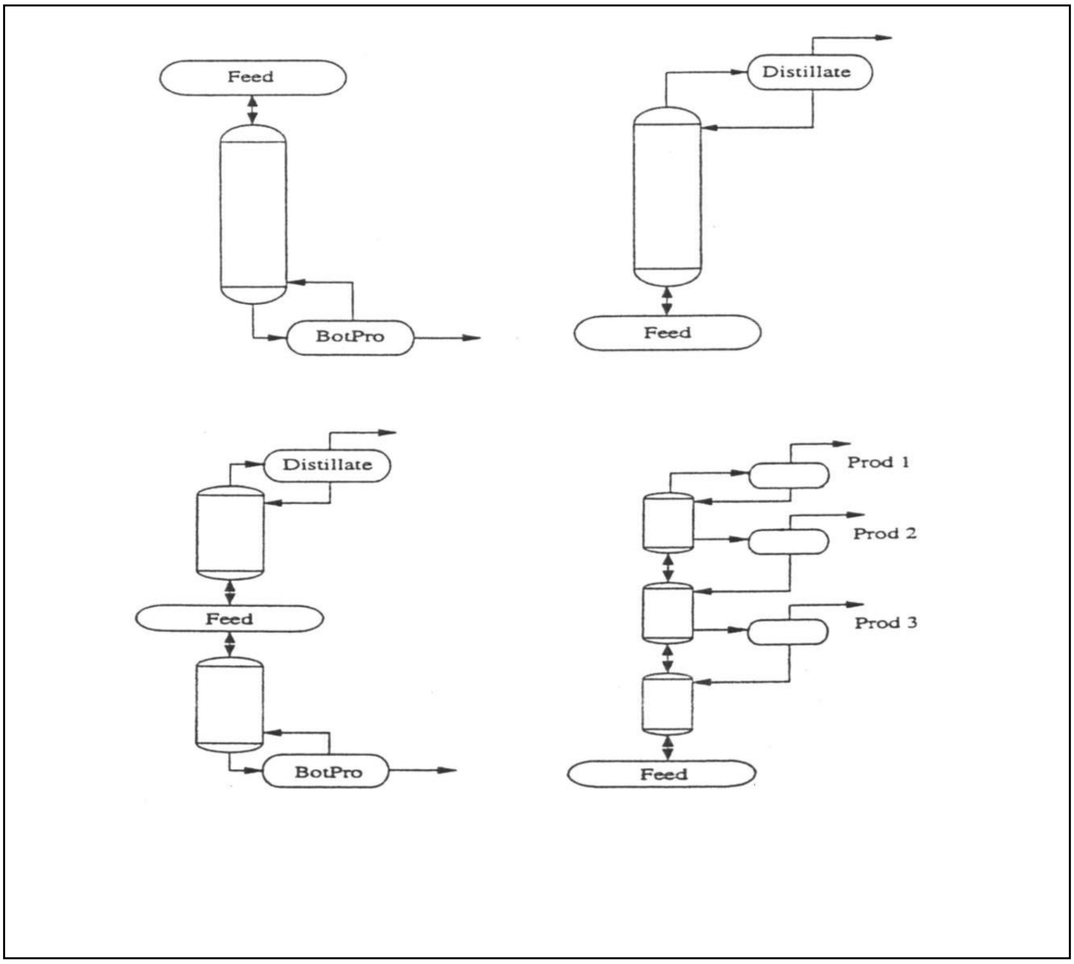

Figure 1.1 Examples of Ways to Configure The Batch Distillation Column.

(Source: Mujtaba.2004)

Current technology has made simulation of a batch distillation much easier and less complicated compared to a few decades. Simulation is usually the first step to conduct feasibility study of a design before it can be implement into a big industrial scale plant. Not only feasibility study, simulation give a better understanding of a process, approximation of the cost to setup and potential challenges that the process may face upon setting up the design to industrial scale.

Graphical method is used to conduct the simulation of process involves in an existing plant. It can help engineers to predict the behaviour of a process using basic engineering relationships such as mass and energy balances, phase and chemical equilibrium, and reaction kinetics. Besides, MATLAB® is also one of alternative software for running this simulation.

1.2 Statement of Project Problem

Simulating the actual operation of convectional column has been the subject of much research for recent century. The main interest was to develop a model that could be the best prediction on batch distillation column. It is difficult to teach batch distillation without using computer because in the process time is varying and has complex numeric integration techniques and process provide flexibility in operating and configuring column.

Batch distillation operates in unsteady where the compositions of the mixture are changing with time. Thus, it is difficult to control the process at all the process. In batch distillation a fixed amount of charge is added to the still for a long time to separate the mixture. Then, top product composition will varies with time. The separation time depends on amount of bottom product composition, number of trays and reflux ratio.

Thus, it needs to consider the ways of configuration based on parameter which needs to be set as basis for a particular design. For a Rigorous model in batch distillation, a detailed analysis of characteristic of differential mass and energy balance associated with the complete dynamics of a multi component (Diweker, 2005). He said that the system of equations presented for batch distillation is more difficult to solve than that for continuous distillation due to several factors.

Simple Rayleigh Model is well- known as the best ways on the modelling of batch distillation (Mujtaba, 2004). It is good with the development of high speed digital computers which is the main issues in modelling. It can detailed energy balances, column holdup, accurate physical properties in order to simulate the actual operation of batch distillation.

In order to verify this issue, simulation of this batch distillation column is to be performed by using computer aided design software and mathematical model so that the results can be compared and validated. It is also necessary to understand the behaviour of batch distillation separation of multi component system.

1.3 Research Objective

Simulation on batch distillation column is done by using computer software simulation to examine the trend of distillate and bottoms composition at constant reflux and regulating reflux for fermentation of product purification. Both of the results from the simulation will be compared to the results obtained experimentally (by others) using an existing column in research study had done by others. Thus, experimental results can be validated.

Secondly is to simulate the parameter of fermentation product purification including reflux ration and column pressure. Here, parameter such as composition product will change with time of separation.

Lastly is to develop a mathematical model in order to study of fermentation product purification.

1.4 Research Questions

1.4.1 Which one the best model of batch distillation process for product purification?

1.4.2 What is the trend of distillate and bottoms composition?

1.4.3 What is the parameter studied that affect the product purification via simulation?

1.5 Scope of Research

In order to achieve the objective of the project, some boundary or scope need to be specified. This project covers the simulation and modelling of separation of fermentation product purification using batch distillation and computer software simulation.

Firstly, the binary mixture used in this project is ethanol-water. It is chosen for it's highly availability and also it is the most common used in the industries, where it is cheap and non-toxic.

Next, this study will focus on comparison the result via simulation and the results obtained experimentally had done by other student.

1.6 Expected Outcomes

This study will be able to examine the trend of distillate and bottoms composition at constant reflux and regulating reflux for fermentation of product purification using batch distillation. These are important results towards the further development of a reference method for product purification. In many cases it was found that the models had to be simplified because of several reasons. There are capabilities of the computer software, availability of suitable numerical methods to integrate the model equations and gain in accuracy of product purity.

It is also expected that high understanding on running the simulation for the industry plant especially using the batch distillation.

1.7 Significance of Research

The most significant input in this study is to increase in the production of high value added, low volume specially chemicals and biochemical for high purity. The research studies highlighted the importance of considering all the design and operational process available in order to gain a comprehensive economical close into the batch distillation process. It is maybe can optimum the production of time, capital costs, mixture characteristic and process allocation. The flexibility of batch distillation processes provides the ability to manage with a market characterized by short product life times and strict specification requirements.

CHAPTER 2

LITERATURE REVIEW

2.1 Introduction

Batch distillation is the oldest separation process which is an important unit operation in the batch processing industry and is widely used (Mujtaba, 2004). The earliest batch distillation is known as Rayleigh distillation, was presented in by Lord Rayleigh (1902). In his model, there is only a condenser, a column and a still pot. No reflux is returned to the still and no stage or packing material inside the column. Hence, Rayleigh distillation is simply a one stage distillation, and the analysis is based on material and component balance (Diwekar, 1996). Due to the increasing of production on high value added, low volume specialty chemicals and biochemical, the batch distillation has been generated a new processing technologies (Diwekar, 1996). The flexibility of batch distillation, combined with inherent unsteady nature of the process, quite challenging design and operation problems. As result, many chemical engineers used batch distillation as their practical in batch processing operation.

2.2 Batch Process

Batch distillation column can be operated with three reflux policies in order to meet certain product specification. The reflux policies that can be employed to a batch distillation are either constant reflux, regulating reflux or optimum reflux. For constant reflux, distillate purity for lighter component will drop over time. In order to maintained the purity of distillate over time, regulating reflux policy can be employed. Optimum reflux policy is used when maximum profit from the operation is required; it is a trade off policy between constant reflux and regulating reflux policies (Diwekar, 1996). In Mujtaba (2004) book states, batch distillation operated on conventional batch distillation and continuous batch distillation.

In conventional batch distillation process, a bottom receiver or reboiler which charged with the feed to be processed and provide the heat transfer surface area. Then, a rectrifying column superimposed on the reboiler, coupled with either a total condenser or partial condenser system. This operation involves carrying out the fractional until desired amount has been distilled. During the process, the overhead composition is varies and usually number of cuts are made. The desired from the cuts are recycling to subsequent batches to obtain further operation.

2.3 Advantages of Batch Distillation

The main advantages of batch distillation based over on a continuous distillation are the uses of single column as opposed to multiple columns and its flexible operation. Besides, the alternative operation does not take into the production of off specification material. Next, only one column and one sequence are necessary to separate all the components in a mixture. Continuous distillation column also can operate for long time (Mujtaba, 2004).

Whereas, Shahidatul (2008) thesis states batch distillation is less energy efficient than continuous distillation and it offers possibility of separating multi-component mixtures into high purity products using single columns. So, it is less expensive compared to continuous distillations that required (n-1) columns. It is flexible and robust to variation in feed composition and specification. It is important for production of seasonal or low capacity chemicals. Batch distillation also can be used for liquids with contaminants such as solids, tars and resins.

2.4 Batch Distillation Operation

Based on Fernholz G. et al., (2000) and Mujtaba (2004), batch distillation is operated in the following manner which is start-up period, production period and shutdown peroid. For start-up, the reboiler is filled with a specified amount of mixture and heated until the complete column is filled with boiling mixture. Then, the manipulated variables in each time interval are set to their optimal values. Lastly, the heat supply and the feed flow are stopped and the system is cooled down. The start-up and shutdown procedures are not included in the optimization because validated models for these phases are not yet available

2.5 Column Configuration

According to Mujtaba (2004) and Diweker (1996), batch distillation column can be operating in various configurations. There are two types of configuration which are conventional column configuration and unconventional column configuration. But, the alternative configuration that has found more advantages is unconventional column distillation. Unconventional configuration consists of inverted batch distillation, middle vessel batch distillation column, multivessel batch distillation column and continuous column. Both writers agree that it is multivessel batch distillation column of configuration to obtain purer product at the of a total reflux operation.

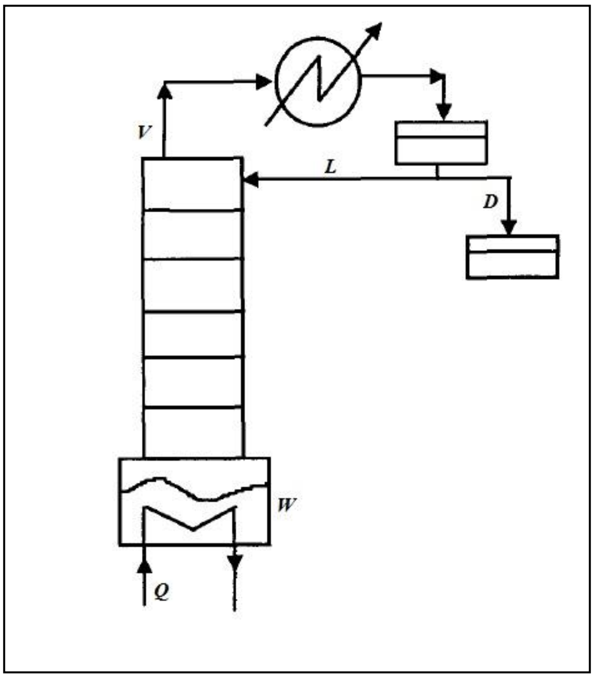

Figure 2.1 Conventional Batch Distillation Column

(Source: Mujtaba, 2004)

2.5.1 An Inverted Batch Column

In this column configuration, the feed mixture is charged into the top reflux drum, and the products are withdrawn at the bottom reboiler. A minimum boiling point azeotrope can be break in inverted batch column compare to the rectifier. Batch time in the inverted column configuration is also better than the regular column for separations where the light component in the feed is present in a small amount. (Diweker, 1996)

Meanwhile, Mujtaba (2004) states in these types, the feed charge and the condenser flux drum are combined and it operates in an all stripping mode with a small holdup reboiler. Its operation is same as the conventional batch column except that products are withdrawn from the bottom. This type of operation is supposed to eliminate the thermal decomposition problem of high boiling point products.

2.5.2 Middle Vessel Column

According to Diweker (1996), this column configuration consists of a middle vessel between two sections of the batch column. The feed is initially charged into the middle vessel, and the products are simultaneously withdrawn from the top and the bottom of the column. The middle vessel column can be an ideal configuration for ternary batch systems. This column configuration is very flexible and effective; hence, it obtains very pure components in the top, bottom, and middle vessel columns.

As mentioned by Mujtaba (2004), in this type, the separation is divided as in the usual continuous distillation column into rectifying and stripping section with a feed tray in the middle. The important features if these types are the feed is supposed to a suitable location in the middle of the column, liquid on the feed tray is recycled to the feed tank and the products can be withdrawn simultaneously from top and bottom of the column. This type is absolutely very flexible in the sense that it can be easily converted to a convectional by changing the location of the feed and by closing or opening appropriate valve in the product.

2.5.3 Multivessel Batch Distillation Column

In this type, the charges in each vessel will be purified as the distillation proceeds if the column operates at total reflux. But, it depends on the number of plates in each section, vapor boil-up, the amount of initial charge in each vessel and the duration of operation to achieve purity (Mujtaba, 2004).

Based on Diweker (1996), this new emerging column configuration can have better separation performance than continuous distillation for systems having a larger number of products. An optimal operation policy for this column can be achieved using variable holdup modes. In this type, the batch time is affected the liquid flow rates in order to minimize distillate than that of the constant holdup mode. Moreover, this column is operated under total reflux conditions. This operation policy can be the ideal operation policy of batch distillation, especially for the middle vessel and multivessel columns. The total reflux mode is commonly used for the last multivessel column because multiple products can be accumulated in each vessel according to their relative volatilities. The initial feed distribution of column performance also been improved using various operating modes in terms of a mean energy consumption rate on the rectifier.

The multivessel column is also studied by Skouras S. & Skogestad S. (2004). This is the first study where the dynamics in the middle vessel of multivessel configurations are discussed where two different of multivessel configurations and a rectifier column are compared to each other .The multivessel batch column can be viewed as a generalization of a batch rectifier and a batch stripper. The column has both a rectifying and a stripping section. Therefore a light and a heavy fraction are possible to obtain simultaneously from the top and the bottom of the column, while an intermediate fraction is also recovered in the middle vessel. In the multivessel column a ternary mixture can be separated simultaneously in one such close operation. No product change-overs are required and all products are accumulated in the three vessels at the end of the process.

2.6 Modelling And Simulation

According to Mujtaba(2004) simulation is the actual operation which consists of simulation of start-up period and simulation of product period. Many research has been done by simulating the operation of convectional column including by Mujtaba(2004), Diweker(1996) and Ronnie (2011). In simulation, it is important to develop a model before run the simulation. The model should consist of mass and energy balance, hydraulic model, physical properties and etc.

Meanwhile, modelling of batch distillation begins with simple Rayleigh Model (Rayleigh, 1902) and the well-known. In modelling, it requires to know whether and how to include energy balance, hydraulic model, accurate physical properties to simulate the actual operation batch distillation. It found that the model had to be simplified first because of size and complexity of the problem, capabilities of computer, and availability of suitable numerical methods to integrate the model equations, gain in accuracy in the prediction of real operation (Mujtaba, 2004).

Mehlhorn et al. (1996) investigated mass transfer and tray hydraulics issues in batch distillation modelling. They have integrated non-equilibrium and equilibrium models to get more accurate model for batch distillation columns with perforated plates. They handled the uncertainties in the mass transfer which was described within the equilibrium-tray model by means of tray efficiency and by using the non-equilibrium-tray model supported by the mass transfer coefficient and the mass transfer area. The developed model was experimentally verified both for binary and multi component systems.

CHAPTER 3

METHODOLOGY

3.1 Computer Software Simulation

Computer software simulation is done by using commercial software (MATLAB ®) and validated using graphical method. MATLAB provides several types of functions for performing mathematical operations and analyzing data, such as matrix manipulation, linear algebra, polynomials and interpolation, ordinary differential equations, partial differential equations, sparse matrix operations, 2D and 3D plotting and much more. The conventional batch distillation that used in this research is simple batch distillation (Rayleigh distillation). In this model, the vapour is removed from the still during a particular time interval and is condensed in the condenser. The more volatile components are richer in the vapour than in the liquid remaining in the still (Diwekar, 2005).